Path integral / Lefschetz thimbles.

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Decompose the integral into steepest descent integrals

$$\int_C d^n x\, e^{-\frac{S(x)}{\hbar}} = \sum_{\sigma:\text{saddles}} \langle K_\sigma, C\rangle \int_{J_\sigma} d^n x\, e^{-\frac{S(x)}{\hbar}}.$$

Motivation

i) Resurgence for exp. integrals:

$$\int_C d^n x\, e^{-\frac{S(x)}{\hbar}} = \sum_{\text{saddles}} \underline{e^{-\frac{S(x_{sad})}{\hbar}}}\, P_{fluc}.$$

Different sectors talk with each other.

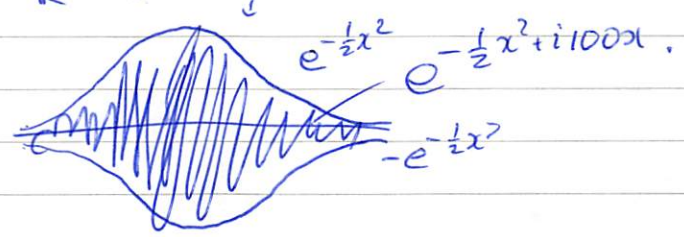
ii) Sign problem.

$$\frac{1}{2}(x-i100)^2 = \frac{1}{2}x^2 - i100x - \frac{10^4}{2}$$

Consider

$$\sqrt{2\pi}\, e^{-10^4/2} = \int_{\mathbb{R}} dx\, \underline{e^{-\frac{1}{2}x^2 + i\cdot 100\, x}}.$$

~~No!~~
~~Numerically~~ ?



~~If we co~~ Take the path through the saddle point $\mathbb{R} \to \mathbb{R}+i100$, then

$$\int_{\mathbb{R}} dx\, e^{-\frac{1}{2}x^2 + i100x} = e^{-10^4/2} \int_{\mathbb{R}} dx\, e^{-\frac{1}{2}x^2}$$

much easier! $\Rightarrow \sqrt{2\pi}$.

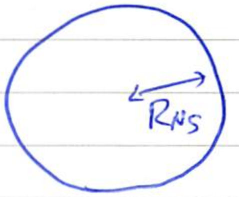
Big Dream: Apply this idea to finite-density QCD!

QCD partition functions:

$$Z = \int \mathcal{D}A\, \underbrace{\mathrm{Det}[\not{D}_A + \mu\gamma^0 - m]}_{\not> 0 \text{ for } \mu \neq 0}\, e^{-S_{YM}[A]}.$$

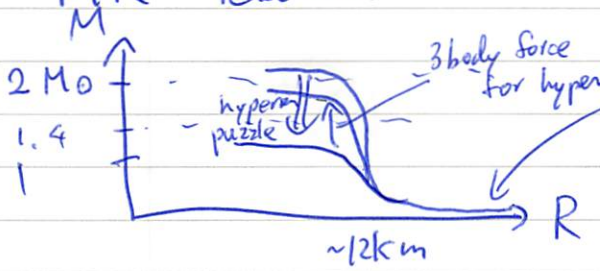
Why are we interested in QCD_μ? ⇒ NS

NS: very small, dense star.
mainly consists of neutrons.

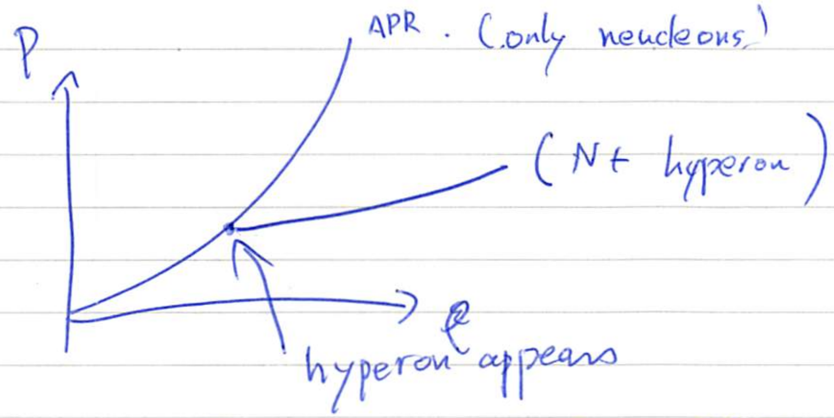


Very big "neucleus" bounded by gravity! $M_{NS} \sim 1.4 M_\odot$
$R_{NS} \sim 12\,km$

MR relation



How can we draw this curve?
- Compute $P = P(\varepsilon)$.
- Solve TOV eq. (hydrostatic + GR).



2010 → 2$M_\odot$ NS!

EOS is more stiff. Can we explain?

1st principle comp. is Necessary!

LATTICE QCD
→ QCD_μ → EOS
↓ few-body physics
Nuclear force
↓ BBG theory
EOS
↓ GR
NS

QCD_μ: Sign problem
⇓
Lefschetz thimble.

Application of Picard-Lefschetz theory to exp. $\int$.
(Picard-Lefschetz theory = complex Morse theory)

Let's understand what

$$\int_{\mathbb{R}^n} d^n x \, e^{-\frac{S(x)}{\hbar}} = \sum_{\sigma \in \Sigma} \langle \mathbb{R}^n, K_\sigma \rangle \int_{J_\sigma} d^n z \, e^{-\frac{S(z)}{\hbar}}$$

means.

$\Sigma = \{ z_\sigma \in \mathbb{C}^n \mid \partial_i S|_{z_\sigma} = 0 \}$.
↑ set of critical points.

$z = x + iy \in \mathbb{C}^n$.

Gradient flow.

$$\frac{dz^i}{dt} = \overline{\left(\frac{\partial S}{\partial z^i}\right)} . \left(= 2 \frac{\partial}{\partial \bar{z}^i} \mathrm{Re} S \right) \quad \left(\frac{dx}{dt} = \frac{\partial \mathrm{Re} S}{\partial x}, \ \frac{dy}{dt} = \frac{\partial \mathrm{Re} S}{\partial y} \right).$$

$\frac{\partial}{\partial \bar{z}^i} = \frac{1}{2}\left(\frac{\partial}{\partial x^i} + \sqrt{-1}\frac{\partial}{\partial y^i}\right)$

Lefschetz thimble (& dual)

$$J_\sigma = \{ z(0) \in \mathbb{C}^n \mid \lim_{t \to -\infty} z(t) = z_\sigma \}. \leftarrow \text{Lefschetz thimble}.$$

$$K_\sigma = \{ z(0) \in \mathbb{C}^n \mid \lim_{t \to +\infty} z(t) = z_\sigma \}.$$

Claim. J_σ, K_σ are n-dim manifolds.

(Assume $z \approx z_\sigma$, then

$S(z) = S(z_\sigma) + \sum_{i=1}^n (z^i - z_\sigma^i)^2$

in appropriate coord. $\mathrm{Re}(S(z) - S(z_\sigma)) = \sum_{i=1}^n \{ (x^i - x_\sigma^i)^2 - (y^i - y_\sigma^i)^2 \}$.

$\Rightarrow$ Locally, $J_\sigma = \{ y^i - y_\sigma^i = 0 \}$
$K_\sigma = \{ x^i - x_\sigma^i = 0 \}$ ← n conditions. $\therefore \dim J = 2n - n = n$.)

Claim For $z \in J_\sigma \cup K_\sigma$,

$$\mathrm{Im}\, S(z) = \mathrm{Im}\, S(z_\sigma).$$

$$\left(\because \frac{d}{dt}(S - \bar{S}) = \frac{\partial S}{\partial z}\frac{dz}{dt} - \frac{\partial \bar{S}}{\partial \bar{z}}\frac{d\bar{z}}{dt} = \frac{\partial S}{\partial z}\overline{\left(\frac{\partial S}{\partial z}\right)} - \frac{\partial \bar{S}}{\partial \bar{z}}\frac{\partial S}{\partial z} = 0 \right)$$

Def. A, B: n-dim mfd $\subset \mathbb{C}^n$. $\langle A, B \rangle = \sum_{p \in A \cap B} (\pm 1)$ ±1 depends on relative orientation

Theorem For nice S,

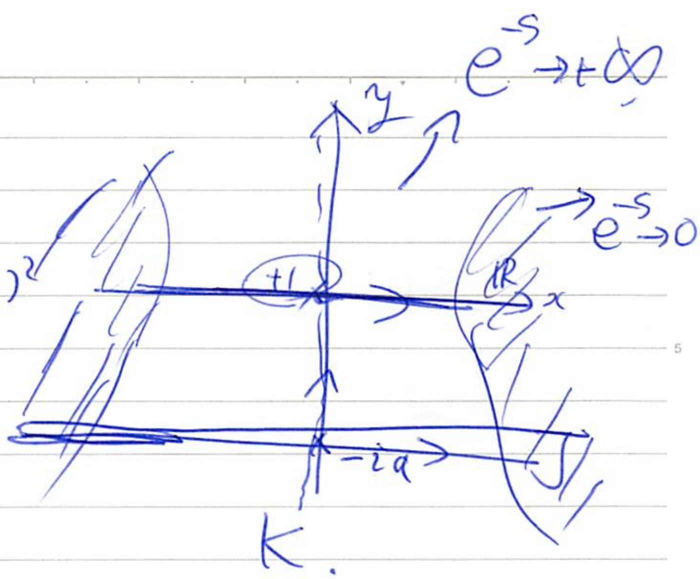
$$\int_{\mathbb{R}^n} d^n x \, e^{-\frac{S(x)}{\hbar}} = \sum_{\sigma \in \Sigma} \langle \mathbb{R}^n, K_\sigma \rangle \int_{J_\sigma} d^n z \, e^{-\frac{S(z)}{\hbar}}.$$

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<u>Gaussian</u> $\int dx \, e^{-\frac{1}{2}(x+ia)^2}$.

$$\int_{\mathbb{R}} dx \, e^{-\frac{1}{2}(x+ia)^2} = \underbrace{\langle \mathbb{R}, K \rangle}_{=1} \int_{J = \mathbb{R} - ia} dx \, e^{-\frac{1}{2}(x+ia)^2}$$

$$= \int_{\mathbb{R}} dx \, e^{-\frac{1}{2}x^2} .$$

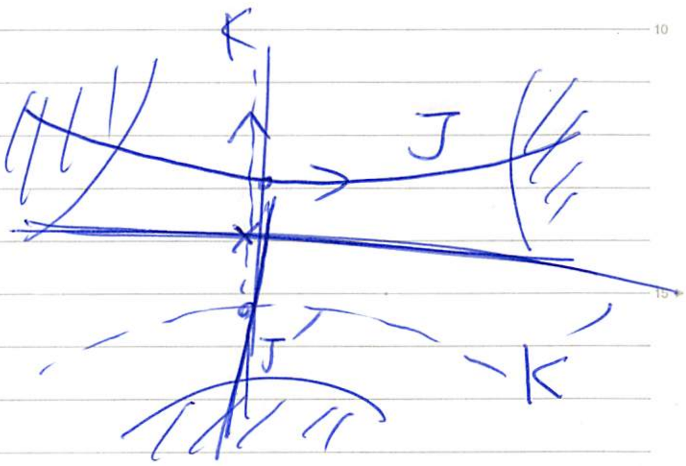


<u>Airy integral</u>

$$\mathrm{Ai}(a) \propto \int_{\mathbb{R}} dx \, e^{i\left(\frac{x^3}{3} + ax\right)}$$

<u>$a = 1$</u>

$$\frac{\partial S}{\partial x} = -i(x^2 + 1) = 0$$



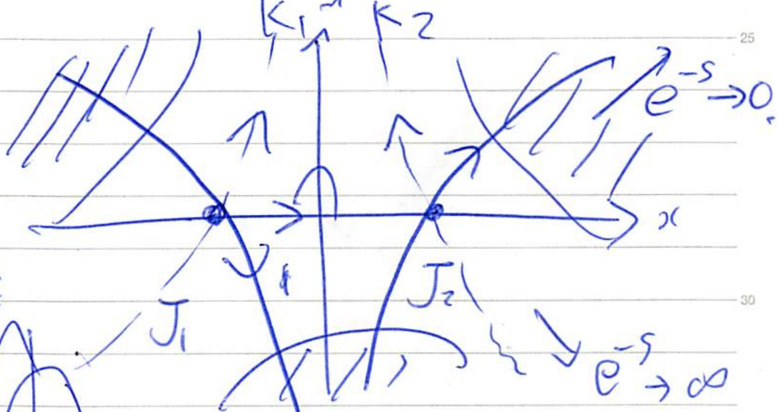
$$\int_{\mathbb{R}} e^{i\left(\frac{x^3}{3} + x\right)} = \underbrace{\langle \mathbb{R}, K \rangle}_{=0} \int_{J} dz \, e^{i\left(\frac{z^3}{3} + z\right)}$$

$$+ \underbrace{\langle \mathbb{R}, K' \rangle}_{=0} \int_{J'} dz \, e^{i\left(\frac{z^3}{3} + z\right)}$$

$$= \int_{J} dz \, e^{i\left(\frac{z^3}{3} + z\right)} . \sim e^{-(@ a^{3/2})}$$

※ This case S is not "nice". Let's discuss it later ...

<u>$a = -1$</u> $\frac{\partial S}{\partial z} = -i(x^2 - 1) = 0$



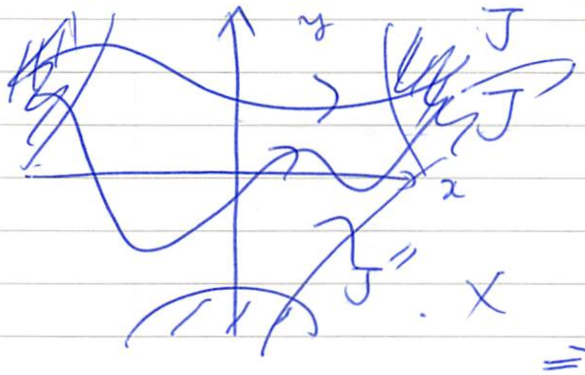
$$\int_{\mathbb{R}} e^{i\left(\frac{x^3}{3} - x\right)}$$

$$= \int_{J_1} dz \, e^{i\left(\frac{z^3}{3} - z\right)} + \int_{J_2} dz \, e^{i\left(\frac{z^3}{3} - z\right)}$$

$$\sim \cos\left(@ a^{3/2} - @\right)$$



Idea of the proof

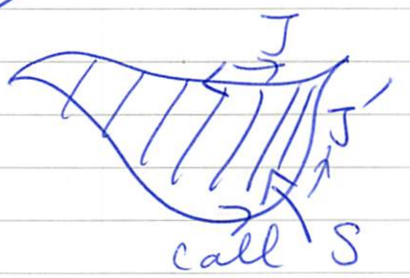


$$\int_J dx\, e^{-S(x)} = \int_{J'} dx\, e^{-S(x)} \neq \int_{J''} dx\, e^{-S(x)}$$

⇒ J and J' must be identified
J ≃ J' and J'' must be distinguished.

~~Let us~~

① Find all possible paths for $\int e^{-S} dx$ without overcounting.



boundary of S,

$$\partial S = J' - J .$$

⇒ If $J - J'$ is a boundary of something, $J \simeq J'$.

• Homology.

Def (Homology). X : m-dim. compact mfd.

$$H_n(X) = \frac{\{A \subset X \mid A : n\text{-dim. submanifold},\ \partial A = \emptyset\}}{\partial\{S \subset X \mid S : (n+1)\text{-dim. submanifold},\ \partial S = \emptyset\}}$$

Def. (Relative Homology) X : m-dim. mfd. Y : n-dim mfd Y ⊂ X.

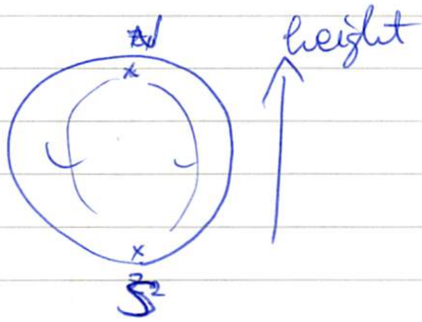
$$H_k(X, Y) = \frac{\{A \subset X \mid A : k\text{-dim. submfd},\ \partial A \subset Y\}}{\partial\{B \subset X \mid B : (k+1)\text{-dim submfd},\ \partial B \subset Y\}}$$

$H_n(\mathbb{C}^n, \{e^{-S} \ll 1\})$ is important for us!

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How to compute $H_n(X)$? $\Rightarrow$ Gradient flow.

Example



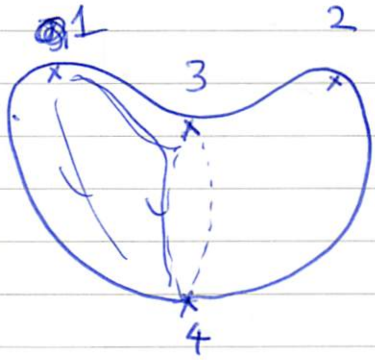
$S = -\text{height}$.

$J_N = S^2$. $\quad J_S = \{S\}$.

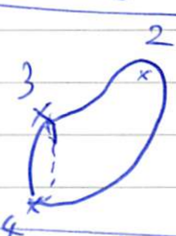
$K_N = \{N\}$, $\quad K_S = S^2$.

$\partial J_N = \emptyset$, $\quad \partial J_S = \emptyset$.

$\Rightarrow H_2(S^2) = \mathbb{R} J_N \simeq \mathbb{R}$, $\quad H_1(S^2) = 0$, $\quad H_0(S^2) = \mathbb{R} J_S \simeq \mathbb{R}$



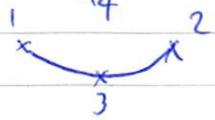
$J_1 =$ 

$J_2 =$ 

$K_1 = \{1\}$, $\quad K_2 = \{2\}$

$J_3 =$ 

$J_4 = \{4\}$.

$K_3 =$ 

$K_4 =$ 

$\partial J_1 = -\partial J_2 = J_3$. $\quad \partial J_3 = 0$, $\quad \partial J_4 = 0$.

$H_2 = \mathbb{R}(J_1 + J_2) \simeq \mathbb{R}$, $\quad H_1 = \dfrac{\mathbb{R}J_3}{\mathbb{R}\partial J_1 \oplus \mathbb{R}\partial J_2} = \dfrac{\mathbb{R}J_3}{\mathbb{R}J_3} = 0$.

$H_0 = \mathbb{R}J_4 \simeq \mathbb{R}$.

KOKUYO

For complex case.

$S(x)$: hol. generic. $\quad \Sigma = \{\frac{\partial S}{\partial x}=0\}$

$$H_n(\mathbb{C}^n; \{e^{-S} \ll 1\}) = \sum_{\sigma\in\Sigma} \mathbb{Z} J_\sigma .$$

$$H_n(\mathbb{C}^n; \{e^{-S} \gg 1\}) = \sum_{\sigma\in\Sigma} \mathbb{Z} K_\sigma .$$

$$H_l(\mathbb{C}^n; \ '' \ ) = \phi \text{ for } l \neq n.$$

($\because$ All J_σ and K_σ are n-dim.)

We've now understood that all possible $\int$ paths are generated by J_σ's.

i.e.

$$\int_{\mathbb{R}^n} d^n x\, e^{-S} = \sum_\sigma n_\sigma \int_{J_\sigma} d^n z\, e^{-S}.$$

↑ What's this? (n_σ)

Intersection pairing:

$$H_n(\mathbb{C}^n, \{e^{-S} \ll 1\}) \otimes H_n(\mathbb{C}^n, \{e^{-S} \gg 1\}) \longrightarrow \mathbb{Z}$$

$$(A, B) \longmapsto \langle A, B\rangle = \sum_{p\in A\cap B} (\pm 1).$$

$\langle J_\sigma, K_\sigma\rangle = 1$. ($\because$ $\forall z \in K_\sigma \setminus \{z_\sigma\}$ $\forall w \in J_\sigma \setminus \{z_\sigma\}$ $\mathrm{Re}\,S(z) > \mathrm{Re}\,S(z_\sigma) > \mathrm{Re}\,S(w)$. $\Rightarrow J_\sigma \cap K_\sigma = \{z_\sigma\}$)

$\sigma \neq \tau \Rightarrow \langle J_\sigma, K_\tau\rangle = 0$ ($\because$ For generic cases, $\mathrm{Im}\,S(z_\sigma) \neq \mathrm{Im}\,S(z_\tau)$, where $\mathrm{Im}\,S(z_\sigma) = \mathrm{Im}\,S(z)$ $\forall z \in J_\sigma$ and $\mathrm{Im}\,S(z_\tau) = \mathrm{Im}\,S(w)$ $\forall w \in K_\tau$.

$\therefore J_\sigma \cap K_\tau = \phi$.)

$[\mathbb{R}^n] = \sum_\sigma c_\sigma [J_\sigma] \in H_n(\mathbb{C}^n, \{e^{-S} \ll 1\})$.

$\langle \mathbb{R}^n, K_\sigma\rangle = \sum_\tau c_\tau \langle J_\tau, K_\sigma\rangle = c_\sigma$. → We got the formula //

Sign problem of QCD_μ, 1-dim. fermion model.

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Review of 1st Lecture

X : n-dim. real affine variety $(= \mathbb{R}^n, SU(N), SO(N), \ldots)$

vol : volume form of X $(= d^n x$, Haar measure, $\ldots)$

S : $\mathbb{C}$-valued polynomial on X, s.t. $\mathrm{Re}\, S(x) \to +\infty$ as $|x| \to \infty$ in X.

Consider

$$\int_X \mathrm{vol}\, e^{-S}.$$

Complexification $X \subset \underset{\text{Kähler mfd.}}{X_{\mathbb{C}}}$ $(= \mathbb{C}^n, SL(N,\mathbb{C}), SO(N,\mathbb{C}), \ldots)$

$$\Rightarrow \begin{cases} \text{Riemannian} & ds^2 = \frac{1}{2} g_{i\bar{j}} (dz^i \otimes d\bar{z}^{\bar{j}} + d\bar{z}^{\bar{j}} \otimes dz^i). \quad (z^i : \text{local coord}) \\ \text{Symplectic} & \omega = \frac{1}{2} g_{i\bar{j}}\, dz^i \wedge d\bar{z}^{\bar{j}} \end{cases}$$

Gradient flow $\overset{\text{Same.}}{\Longleftrightarrow}$ Hamilton eq.

$$\frac{dz^i}{dt} = g^{i\bar{j}} \partial_{\bar{j}} \bar{S}, \qquad \frac{d}{dt} z^i = \{\mathrm{Im}\, S, z^i\}_{\text{Poisson}}.$$

$\Downarrow$ $\mathrm{Re}\, S$ monotonically increases. $\Downarrow$ $\mathrm{Im}\, S$ conserved.

$\Sigma = \{\nabla S = 0\}$.

$J_\sigma = \{ z(0) \mid z(t) \xrightarrow{t \to -\infty} z_\sigma \}$, $K_\sigma = \{ z(0) \mid z(t) \xrightarrow{t \to +\infty} z_\sigma \}$.

Then, If S is "nice" (Morse-Smale, no saddles at ∞),

$$\int_X \mathrm{vol}\, e^{-S} = \sum_{\sigma \in \Sigma} \langle X, K_\sigma \rangle \int_{J_\sigma} \mathrm{vol}\, e^{-S}.$$

To relate this formula with the Borel sum, consider

$$\gamma_\sigma^t := \{ z \in J_\sigma \mid \mathrm{Re}\,(S(z) - S(z_\sigma)) = t \},$$

and use the equality

$$\int_{J_\sigma} \mathrm{vol}\, e^{-S} = e^{-S(z_\sigma)} \int_0^\infty dt\, e^{-t} \underbrace{\int_{\gamma_\sigma^t} \left[\frac{\mathrm{vol}}{dS|_t}\right]} \qquad \left(\mathrm{vol} = dS_t \wedge \left[\frac{\mathrm{vol}}{dS_t}\right]\right).$$

(Check Nevalinna criterion) $= B$[Perturbative series around z_σ]

$$\begin{cases} \text{Stokes constants} & \to \text{ jump of } \langle X, K_\sigma \rangle. \\ \text{Stokes line} & \to \exists \sigma \neq \tau \quad \mathrm{Im}\, S(z_\sigma) = \mathrm{Im}\, S(z_\tau) \\ \text{Anti-Stokes line} & \to \exists \sigma \neq \tau \quad \mathrm{Re}\, S(z_\sigma) = \mathrm{Re}\, S(z_\tau) \end{cases}$$

※ S is assumed to be very "nice".

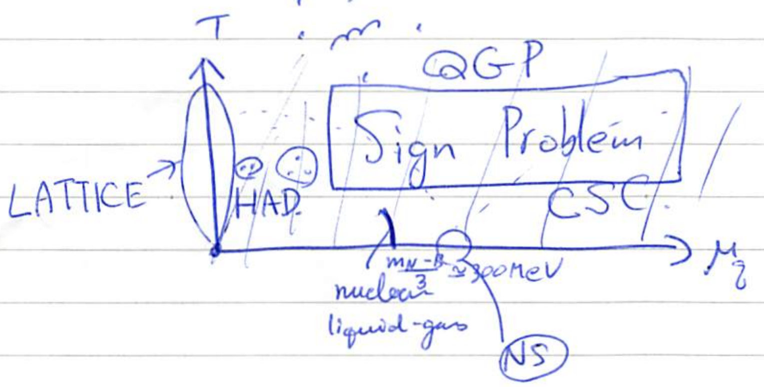
Sign problem of QCD_μ

$$Z = \int \mathcal{D}A \; \mathrm{Det}[\not{D}_A - \mu\gamma^0 + m] \, e^{-S_{YM}[A]}.$$

- $(\not{D}_A)^\dagger = -(\not{D}_A)$. $\quad \{\gamma_5, \not{D}_A\} = 0$.
  - $\Rightarrow$ Spectrum of $\not{D}_A \subset i\mathbb{R}$, and form pairs $\pm i\lambda_n$.
  - $\Rightarrow$ At $\mu = 0$

$$\mathrm{Det}[\not{D}_A + m] = \prod_n (\lambda_n^2(A) + m^2) > 0.$$

- Anti-Hermiticity is lost at $\mu \neq 0$.



Silver Blaze problem

Consider $\lim_{T\to 0} Z_{QCD}(T,\mu) = Z_{QCD}(T=0,\mu)$.
For $0 < \mu < \frac{m_N - B}{3}$,

$$Z(T=0,\mu) = Z(T=0, \mu=0).$$

Show it.

"Easy" part: $0 < \mu < \frac{m_\pi}{2}$.
Compute $Z_{QCD}(0,\mu)$ as

$$Z(0,\mu) = \int \mathcal{D}A \; \mathrm{Det}[\not{D}_A + m] \, e^{-S_{YM}[A]} \, \frac{\mathrm{Det}[\not{D}_A - \mu\gamma^0 + m]}{\mathrm{Det}[\not{D}_A + m]}.$$

i.e.

$$\frac{Z(0,\mu)}{Z(0,0)} = \left\langle \frac{\mathrm{Det}[\not{D}_A - \mu\gamma^0 + m]}{\mathrm{Det}[\not{D}_A + m]} \right\rangle_{T=0,\mu=0}.$$

· Dimensionally-reduced expression.

Consider

$$\gamma^0(\not{D}_A - \mu\gamma^0 + m) = \partial_\tau - iA^0 + \gamma^0 \not{D}_{A,i} + \gamma^0 m - \mu .$$

instead of $\not{D}_A - \mu\gamma^0 + m$.

$$\mathrm{Spec}(\gamma^0 \not{D}_A + m) =: \{\lambda_{j,n}\}_n .$$

where (KK) ← Matsubara freq.

$$\lambda_{j,n} = \varepsilon_j(A) + i\phi_j(A) + (2n+1)i\pi T .$$

$$\mathrm{Det}[\not{D}_A - \mu\gamma^0 + m] = \text{``}\prod_{j,n}(\lambda_{j,n} - \mu)\text{''}$$

$$= N(A) \prod_{\varepsilon_j > 0} \left(1 + e^{-\beta(\varepsilon_j + i\phi_j - \mu)}\right) \quad \leftarrow \text{quark}$$

$$\times \left(1 + e^{-\beta(\varepsilon_j - i\phi_j + \mu)}\right) . \quad \leftarrow \text{anti-quark}$$

Therefore,

$$\frac{\mathrm{Det}[\not{D}_A - \mu\gamma^0 + m]}{\mathrm{Det}[\not{D}_A + m]} = \prod_{\varepsilon_j > 0} \frac{\left(1 + e^{-\beta(\varepsilon_j + i\phi_j - \mu)}\right)\left(1 + e^{-\beta(\varepsilon_j + i\phi_j + \mu)}\right)}{\left(1 + e^{-\beta(\varepsilon_j + i\phi_j)}\right)\left(1 + e^{-\beta(\varepsilon_j + i\phi_j)}\right)}$$

$$\xrightarrow{\beta \to \infty} 1 \quad \text{for } 0 < \mu < \min_{\varepsilon_j > 0}(\varepsilon_j) .$$

$$\min_{\varepsilon_j > 0}(\varepsilon_j) = m_\pi / 2 .$$

(∵) The same logic applies for μ_I.
In this case $\mu_I = m_\pi/2$ is the critical value.

"Difficult" part: $\frac{m_\pi}{2} < \mu < \frac{m_N - B}{3}$.

· Totally unknown.

· At each gauge config. at $\mu = 0$, pion condensation occurs

i.e. $\langle \pi^+ \rangle(A) \neq 0$ for $\mu > m_\pi/2$.

This must be killed by the ensemble average of A.

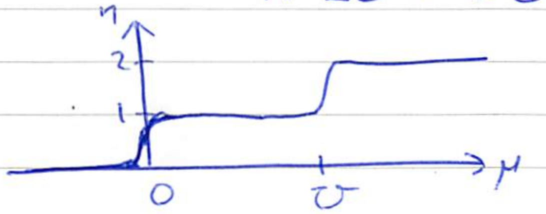
(0+1)-dim. fermion model & Silver Blaze problem

One-site Hubbard model:

$$\hat{H} = U \hat{n}_\uparrow \hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow), \quad (\hat{n}_\sigma = \hat{c}^+_\sigma \hat{c}_\sigma).$$

This is 4-level QM.

$$\langle \hat{n}_\uparrow + \hat{n}_\downarrow \rangle = \frac{2(e^{\beta\mu} + e^{\beta(2\mu - U)})}{1 + 2e^{+\beta\mu} + e^{-\beta(U-2\mu)}}$$



$T/U \ll 1.$

Lagrangian:

$$S_{eff} = \int_0^\beta d\tau \left[\psi^+ \left(\partial_\tau - (\mu + \frac{U}{2}) - i\phi\right)\psi + \frac{\phi^2}{2U}\right]. \quad (\mathrm{Im}\langle\phi\rangle / U = n).$$

$$Z = \int \mathcal{D}\phi \, e^{-\int_0^\beta d\tau \frac{\phi^2}{2U}} \underbrace{\mathrm{Det}\left[\partial_\tau + \mu + \frac{U}{2} - i\phi\right]}$$

dimensionally-reduced expression

$$= \left(1 + e^{-\beta(\frac{U}{2} - \mu - i\varphi)}\right)^2.$$

$$\left(\varphi = \frac{1}{\beta}\int_0^\beta d\tau\, \phi, \quad \lambda_n = -\frac{U}{2} - i\varphi + (2n+1)\pi i T\right).$$

$$= \sqrt{\frac{\beta}{2\pi U}} \int d\varphi \, e^{-\frac{\beta}{2U}\varphi^2 + \ln\left[1 + e^{-\beta(\frac{U}{2} - \mu - i\varphi)}\right]^2}$$

origin of the sign problem. (↑ pointing at i)

> • Silver Blaze Problem of 1-site Hubbard model
> Show that $Z(T=0, \mu) = Z(T=0, \mu=-\infty)$ for $\mu < 0$.

·) Easy part: For $\mu < -\frac{U}{2}$, then for any $n \in \mathbb{Z}$.

$$\mathrm{Re}(\lambda_n - \mu) = -\mu - \frac{U}{2} > 0.$$

This means that $\mathrm{Det}[(\partial_\tau + \frac{U}{2} + i\phi) + \mu] = (1 + e^{-\beta(-\frac{U}{2} - \mu - i\varphi)})^2 \xrightarrow{\beta \to \infty} 1.$

Then, Sign Problem is "exponentially weak" at $T \to 0$.

·) Difficult part: $-\frac{U}{2} < \mu < 0$.

Let's understand the Sign Problem of this model w/ Lefschetz thimbles.

$$S(\phi) = \frac{\beta}{2U}\phi^2 - 2\ln\left[1+e^{-\beta(-\frac{U}{2}+i\phi-\mu)}\right]$$

Classical eom:

$$0=\frac{\partial S}{\partial \phi} \iff i\phi = -\frac{2U}{1+e^{-\beta(i\phi+\mu+\frac{U}{2})}}.$$

- For $\mu < -\frac{U}{2}$, $\phi = 0$ satisfies eom with exponential accuracy. Indeed,

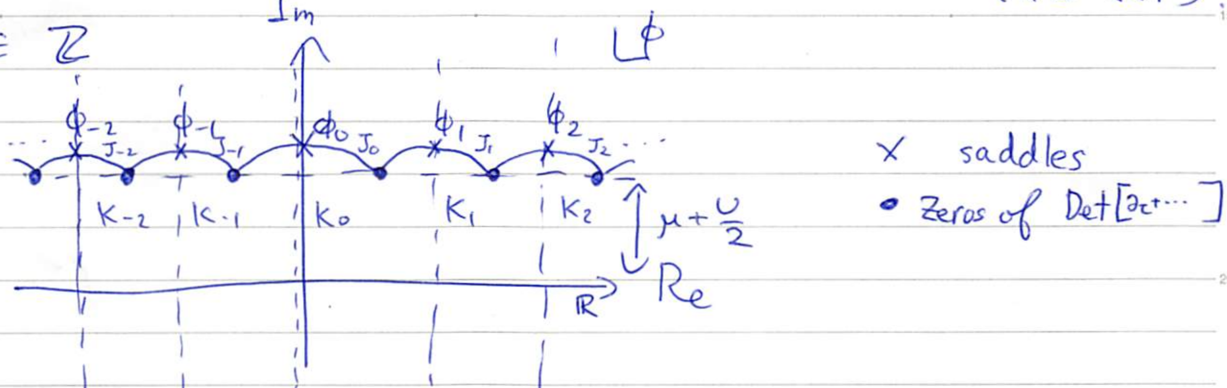
$$n = \mathrm{Im}\langle\phi\rangle/U \simeq 0.$$

- $-\frac{U}{2} < \mu \ \left(< \frac{3U}{2}\right)$

$$\phi_m = i\left(\mu+\frac{U}{2}\right) + T\left(2\pi m + i\ln\frac{\frac{3}{2}U-\mu}{\frac{1}{2}U+\mu}\right) + O(T^2)$$

$(T/U \ll 1)$

w/ $m \in \mathbb{Z}$



$\Rightarrow \langle \mathbb{R}, K_m\rangle = 1$ for all $m\in\mathbb{Z}$.

$$Z = \sqrt{\frac{\beta}{2\pi U}}\int_{\mathbb{R}} d\phi\, e^{-S(\phi)} = \sqrt{\frac{\beta}{2\pi U}}\sum_{m\in\mathbb{Z}}\int_{J_m} d\phi\, e^{-S(\phi)}.$$

To find an impact of $\sum_m$, let's simplify Z as

$$Z \Rightarrow Z' = \sum_{m\in\mathbb{Z}} e^{-S(\phi_m)} = e^{-S(\phi_0)}\sum_{m\in\mathbb{Z}} e^{-(S(\phi_m)-S(\phi_0))};$$

where

$$S(\phi_0) = -\beta\cdot\frac{U}{2}\left(\frac{\mu}{U}+\frac{1}{2}\right)^2 \quad (= -\beta\cdot(\text{mean-field free energy})).$$

$$S(\phi_m) - S(\phi_0) = \frac{2\pi^2}{\beta U}m^2 + 2\pi i\, m\left(\frac{\mu}{U}+\frac{1}{2}\right) + ~~O(T)~~.$$

at low temperatures.

Therefore,

$$Z' = e^{\frac{\beta U}{2}\left(\frac{\mu}{U}+\frac{1}{2}\right)^2} \sum_m e^{-\frac{1}{2}\frac{(2\pi m)^2}{\beta U} - 2\pi i m\left(\frac{\mu}{U}+\frac{1}{2}\right)}$$

$$= e^{\frac{\beta U}{2}\left(\frac{\mu}{U}+\frac{1}{2}\right)^2} \sqrt{\frac{\beta U}{2\pi}} \sum_\ell e^{-\frac{1}{2}\frac{\beta U}{(2\pi)^2}\left(2\pi\left(\frac{\mu}{U}+\frac{1}{2}\right)-2\pi\ell\right)^2}$$

(Poisson summation formula)

$$\underbrace{\left(2\pi\left(\frac{\mu}{U}+\frac{1}{2}\right)-2\pi\ell\right)^2}_{=\,(2\pi)^2\left(\frac{\mu}{U}+\frac{1}{2}-\ell\right)^2}$$

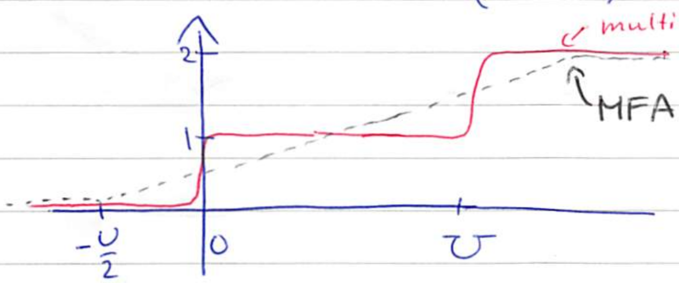
$\Rightarrow$ $\ell = 0$ is important for $0 < \frac{\mu}{U}+\frac{1}{2} < \frac{1}{2}$.
$\ell = 1$ is important for $\frac{1}{2} < \frac{\mu}{U}+\frac{1}{2} < \frac{3}{2}$
⋮

That is,

$$F' = -\frac{1}{\beta}\ln Z' \simeq \begin{cases} 0 & \left(-\frac{U}{2} < \mu < 0\right) \\ -\mu & (0 < \mu < U) \end{cases}$$

and

$$n = \begin{cases} 0 & \left(-\frac{U}{2} < \mu < 0\right) \\ 1 & (0 < \mu < U) \end{cases}$$



In the "Difficult" Silver Blaze region, there's a BIG impact of interference among multiple Lefschetz thimbles.

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About simulations of LATTICE FIELD THEORY

- Goal: Evaluate

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, e^{-S[\phi]} \, \mathcal{O}[\phi]$$

numerically for observables $\mathcal{O}$. "∞-dim." integral.

$$S[\phi] = \int d^4x \left[\frac{1}{2}(\partial\phi)^2 + V(\phi) \right]$$
$$\Rightarrow a^4 \sum_{x\in\Lambda} \left[\frac{1}{2} \sum_{i=1}^{4} \left(\frac{\phi(x+ae_i) - \phi(x-ae_i)}{2a}\right)^2 + V(\phi(x)) \right].$$

$$\int \mathcal{D}\phi \Rightarrow \prod_{x\in\Lambda} \int d\phi(x).$$

$\Lambda \subset (a\mathbb{Z})^4 \subset \mathbb{R}^4$. $a \to 0 \Rightarrow (a\mathbb{Z})^4$ is "good approx." of $\mathbb{R}^4$.

Direct ~~numerical~~ comp. $\mathcal{O}(\#^{|\Lambda|})$ ($\#$ = cost of each $\int d\phi(x)$)

$\Rightarrow$ Monte Carlo integration.

- Importance Sampling

$$\text{Integrand} = \frac{1}{Z} e^{-S[\phi]} \times \mathcal{O}$$

$e^{-S[\phi]}$: Boltzmann factor, $S[\phi] \propto |\Lambda| a^4 = \text{volume}$; $\mathcal{O}$: Observables

$\Rightarrow$ Full field space is unimportant.

(For a moment, assume $S[\phi] \in \mathbb{R}$.)

Most configs ϕ are exponentially suppressed, $\mathcal{O}(e^{-\text{volume}\,\#})$.

Efficient numerical method should pay attention mainly to regions (entropy for similar configs) $\times e^{-S}$ ~~≪1~~.

- Generate $\{\phi_n\}_{n=1}^{\infty}$ obeying $P_{eq}[\phi] = \frac{1}{Z} e^{-S[\phi]}$, then

$$\langle \mathcal{O} \rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}(\phi_n).$$

How to generate sequences $\{\phi_n\}_n$ obeying $P_{eq} \propto e^{-S}$?

Update configs ϕ stochastically.

- Transition probability $P(\phi_j \to \phi_i)\,(=: P_{ij})$

If $P(\phi_j \to \phi_i)$ satisfy

(Detailed Balance) $\quad P(\phi \to \phi')\, P_{eq}[\phi] = P(\phi' \to \phi)\, P_{eq}[\phi']$

&

(Strong Ergodicity) $\quad P(\phi \to \phi') > 0$,

then the sequence $\{\phi_n\}_{n=1}^{\infty}$ obtained by this update

obeys P_{eq} for $n \gg 1$.

Proof. (SE) says $P_{ij} > 0$ for all ij.

$\Rightarrow$ Perron-Frobenius says $(P_{ij})_{ij}$ has the unique maximal eigenvalue, 1, and eigenvector: $\tilde{P}_{eq}$.

$$\sum_{\phi'} P(\phi' \to \phi)\, {}^{\exists!}\tilde{P}_{eq}(\phi') = \tilde{P}_{eq}(\phi).$$

$\tilde{P}_{eq} = P_{eq}$, because

$$\sum_{\phi'} P(\phi' \to \phi)\, P_{eq}(\phi') \overset{(DB)}{=} \underbrace{\sum_{\phi'} P(\phi \to \phi')}_{=1} P_{eq}(\phi) = P_{eq}(\phi). \quad //$$

$$\left(\text{i.e.} \quad P_{eq} = \lim_{k \to \infty} \sum_{\phi_1, \ldots, \phi_k} \underbrace{{}^{\forall}P_{initial}[\phi_1]}_{\geq 0} P(\phi_1 \to \phi_2)\, P(\phi_2 \to \phi_3) \cdots P(\phi_k \to \phi) \right)$$

Let us show three examples :

1) Metropolis method

Pick up a trial transition probability, P_{trial}, satisfying

$$P_{trial}(\phi \to \phi') = P_{trial}(\phi' \to \phi). \ (>0),$$

(i) Suggest a new config. ϕ' according to $P_{trial}(\phi \to \cdot)$.

(ii) $e^{-S(\phi')} > e^{-S(\phi)} \Rightarrow$ Accept ϕ'.

$e^{-S(\phi')} \leq e^{-S(\phi)} \Rightarrow$ Accept ϕ' with the probability $e^{-(S(\phi')-S(\phi))}$.

(DB) ✓.

Typically, only good for local updates.
update $\phi(x)$ for each x successively.

(Assume $e^{-S(\phi)} \sim 1$.
If one proposes $\phi_{new} = \{\phi_{new}(x)\}_{x\in\Lambda}$ for all x randomly
$S(\phi_{new}) \gg S(\phi)$. ($S(\phi_{new}) - S(\phi) \sim \#|\Lambda|$).
ϕ_{new} will never be accepted.)

2) Langevin method.

Introduce the stochastic time θ, and consider

$$\frac{d\phi(x,\theta)}{d\theta} = -\frac{\partial S}{\partial \phi(x,\theta)} + \eta(\theta).$$

$\eta(\theta)$: white noise $\begin{cases} \langle \eta(\theta) \rangle = 0 \\ \langle \eta(\theta)\eta(\theta') \rangle = 2\delta(\theta-\theta') \end{cases}$

(DB) ✓ , (Global update) ✓.

↳ BUT, this is true ONLY for the conti. limit of θ.

($\Rightarrow$ Origin of systematic error).

3) Hybrid Monte Carlo (HMC) method.

- Metropolis test ⇒ (DB) is exactly satisfied.
- Proposal of ϕ_{new} using differential eqs. ⇒ Global update.

Notice the trivial equality:

$$\langle \mathcal{O}[\phi] \rangle = \frac{1}{Z}\int \mathcal{D}\phi \, e^{-S[\phi]} \mathcal{O}[\phi]$$
$$= \frac{1}{Z'}\int \mathcal{D}\phi \mathcal{D}\pi \, e^{-\left[\int d^dx \frac{\pi^2}{2} + S[\phi]\right]} \mathcal{O}[\phi].$$

π: new field, canonical momentum of ϕ.

$H[\phi,\pi] := \int d^dx \frac{\pi(x)^2}{2} + S[\phi]$: Hamiltonian

Propose ϕ_{new} by solving molecular dynamics (MD),

$$\frac{d\phi}{d\theta} = \{H, \phi\}, \quad \frac{d\pi}{d\theta} = \{H, \pi\}. \quad \text{(MD)}$$

(i) Choose an initial config. $\{\phi(x)\}_x$
(ii) Pick up $\{\pi(x)\}_x$ according to $\propto e^{-\int d^dx \frac{\pi(x)^2}{2}}$.
(iii) Solve (MD) for a certain time interval $\Delta\theta$ with the initial cond. $\{\phi(x), \pi(x)\}_x$.
Call the final result as $\{\phi', \pi'\}$.
(iv) Accept $\{\phi', \pi'\}$ according to $P = \mathrm{MIN}\{1, \exp[-(H[\phi',\pi'] - H[\phi,\pi])]\}$
Repeat.

(DB) ✓, (Global update) ✓.

* So far, $S[\phi]$ is assumed to be real.

What happens if $S[\phi] \in \mathbb{C}$?

1), 3). Metropolis test says ϕ' should be accepted with $p = \mathrm{MIN}\{1, \exp\{-(S[\phi'] - S[\phi])\}$ $\in \mathbb{C}$?.

Historically, 2) gets much attention since there is no Metropolis test.
$\Rightarrow$ Complex Langevin method.

$\phi \in \mathbb{R} \to z \in \mathbb{C}$.

$$\frac{dz}{d\theta} = -\left(\frac{\partial S}{\partial z}\right) + \eta(\theta).$$

- Correct perturbative series.
- Sometimes works, but sometimes doesn't.
- (DB) is unknown, i.e. $P_{eq}^{(CL)}$ is unknown.

Assuming
- Semiclassical approx. is good, and
- There are several saddles z_σ with $\langle \mathbb{R}, K_\sigma \rangle \neq 0$ and $\mathrm{Re}(S_\sigma)$ are same and minimal, and $\mathrm{Im}\, S_\sigma \neq \mathrm{Im}\, S_\tau$.

we can "prove" CL is wrong.

"Proof"

$$\langle \mathcal{O}[z] \rangle_{CL} = \int dz d\bar{z}\, P_{eq}^{(CL)}(z, \bar{z})\, \mathcal{O}(z) \simeq \sum_\sigma^{\exists} \underset{>0}{c_\sigma}\, \mathcal{O}(z_\sigma)$$

>0, should localize around z_σ's

$\|$ "If CL is correct"

$$\frac{1}{Z}\int_{\mathbb{R}} d\phi\, e^{-S(\phi)} \mathcal{O}(\phi) = \sum_\sigma \langle \mathbb{R}, K_\sigma \rangle \int_{J_\sigma} dz\, e^{-S(z)} \mathcal{O}(z) \simeq \frac{1}{Z} \sum_\sigma \frac{\langle \mathbb{R}, K_\sigma \rangle}{\sqrt{2\pi S''(z_\sigma)}} e^{-S(z_\sigma)} \mathcal{O}(z_\sigma)$$

- For dominant σ's, they equally contribute with different complex phases.

- Positivity of $P_{eq}^{(CL)}$ says $c_\sigma > 0$. $\Rightarrow$ Contradiction //.

$\gtrsim 2012$, Lefschetz-thimble techniques are introduced to the sign problem

$$\int_{C_{\mathbb{R}}} \mathcal{D}\phi\, e^{-S[\phi]} \mathcal{O}(\phi) = \sum_{\sigma\in\Sigma} \langle C_{\mathbb{R}}, K_\sigma \rangle \int_{J_\sigma} \mathcal{D}\phi\, e^{-S}\, \mathcal{O}(\phi)$$

$$= \sum_{\sigma\in\Sigma} \langle C_{\mathbb{R}}, K_\sigma \rangle e^{-i\,\mathrm{Im}(S_\sigma)} \int_{J_\sigma} \mathcal{D}\phi\, e^{-\mathrm{Re}(S)}\, \mathcal{O}(\phi).$$

- Lefschetz thimble is defined by the flow

$$\frac{d\phi(x,t)}{dt} = \overline{\left(\frac{\partial S}{\partial \phi(x,t)}\right)}.$$

$\Rightarrow$ Local update does not make sense.

In 1), 2), 3), 2) Langevin & 3) HMC does not rely on local updates.

- Langevin on thimbles (Aurora-algorithm)
- HMC ——
(: Parma method / contraction algorithm).

- Aurora-algorithm

Pick up a thimble J_0, and try to compute

$$\langle \mathcal{O}(\phi)\rangle_0 := \frac{1}{Z_0} e^{-i\,\mathrm{Im}\,S_0} \int_{J_0} \underbrace{\mathcal{D}\phi}_{=|\mathcal{D}\phi|\cdot(\text{Jacobian})} e^{-\mathrm{Re}\,S(\phi)}\, \mathcal{O}(\phi), \left(\overset{?}{=} \frac{e^{-S_0}}{Z_0} \int_0^\infty dt\, e^{-t} \underbrace{\int_{\Gamma_0^t} \left[\frac{\mathcal{D}\phi}{dS}\right] \mathcal{O}(\phi)}_{=\mathcal{B}[\text{perturbation}]} \right)$$

Langevin eq.

$$\begin{cases} \frac{d}{d\theta}\phi^{(R)} = -\frac{\partial}{\partial\phi^{(R)}}\mathrm{Re}\,S + \eta^{(R)}(\theta) \\ \frac{d}{d\theta}\phi^{(I)} = -\frac{\partial}{\partial\phi^{(I)}}\mathrm{Re}\,S + \eta^{(I)}(\theta). \end{cases}$$

(the boxed noise term $\in T_\phi J_0$.)

To prepair the noise η, we must know tangent space $T_\phi J_0$.

$\Rightarrow$ Take the deviation of flow eq:

$$\frac{d}{dt}\delta z = \overline{\left(\frac{\partial^2 S}{\partial\phi\,\partial\phi}\right) \delta z}.$$

$\Rightarrow$ Project the stochastic noize along each tangent space.

$\Rightarrow$ Reweight the Jacobian factor.

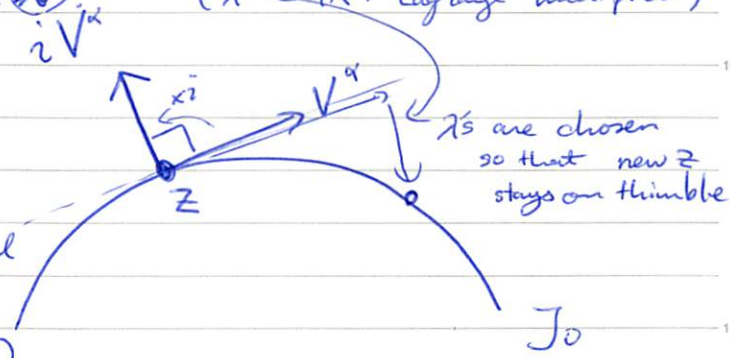
- HMC on Lefschetz thimbles

1) Generate a Lefschetz thimble J_0 including tangential directions, i.e. $TJ_0 = \{ (z, \{V_z^\alpha\}_\alpha) \}$.

2) Formulate MD:
Define the classical ~~EOM~~ dynamics constrained on the Lefschetz thimble:

$$\frac{d}{dt} z_i = w_i$$
$$\frac{d}{dt} w_i = -\overline{\partial_i}\,\overline{S} - i\, V_{z\,i}^{\alpha} \lambda^\alpha \quad (\lambda^\alpha \in \mathbb{R} : \text{Lagrange multipliers})$$

Constraints:
$(z_i, w_i) \in TJ_0$
$\quad\;\; \Vert$
$V_i^\alpha w^\alpha \in \mathbb{R}$.



This dynamics has a conserved Hamiltonian:
$$H = \frac{1}{2}\bar{w}_i w_i + \frac{1}{2}\left(S[z] + \overline{S[z]}\right).$$

3) HMC i) Generate an initial config. $z \in J_0$
ii) Refresh the momentum $w = V^\alpha w^\alpha$ by generating w^α in appropriate random way.
iii) Solve MD.
iv) Do Metropolis test by $H[z', w'] - H[w, z]$.
Repeat.

⇒ Reweight with the Jacobian factor, which gives $\langle O[\phi] \rangle_0$.

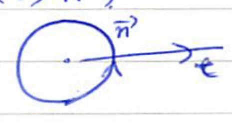
- Other possibilities

* Parma method 1: Use the fact that $J_0 \setminus \{z_0\} \simeq \mathbb{R} \times S^{n-1}$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (t, \vec{n})$

Decompose $\int_{J_0} \mathcal{D}\phi(\cdots)$ as
$$\int d\vec{n} \int dt\, (\cdots)'.$$

Do crude MC for $\vec{n}$ integrals.

dim $(\vec{n} = 2)$



* Parma method 2: Assume that $J_0 \simeq T_0 J_0$ ← flat space.
In this case, we need not care about difficulties of the flow eq.
⇒ Local update is possible. Apply heat-bath, etc.

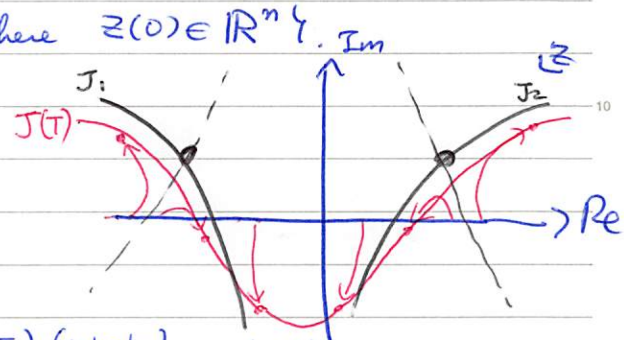
- Contraction algorithm, Beyond thimbles

In 2^{nd} Lecture, we've learned that it's impossible to kill the sign problem completely when there's difficult Silver Blaze.

$\Rightarrow$ Compromise with milder sign problem, then we do not need to stay on thimbles.

Gradient flow: $\frac{dz}{dt} = \overline{\left(\frac{\partial S}{\partial z}\right)}$.

$$J(T) := \{ z \in \mathbb{C}^n \mid z(T) = z, \text{ where } z(0) \in \mathbb{R}^n \}.$$



$[J(T)] = [\mathbb{R}^n]$ in $H_n(\mathbb{C}^n, \{e^{-S} \ll 1\})$, and thus

$$\int_{\mathbb{R}^n} d^n x\, e^{-S(x)} = \int_{J(T)} d^n z\, e^{-S(z)}.$$

We can construct the map $\mathbb{R} \to J(T)$ (U(1)) explicitly as

$$\begin{array}{ccc} \mathbb{R} & \longrightarrow & J(T) \\ \rotatebox{90}{$\in$} & & \rotatebox{90}{$\in$} \\ x & \longmapsto & z(T, x), \end{array}$$

where

$$\frac{dz(t,x)}{dt} = \overline{\left(\frac{\partial S}{\partial z}\right)}, \quad z(0,x) = x.$$

Now, we get

$$\begin{aligned} \int_{\mathbb{R}^n} d^n x\, e^{-S(x)} &= \int_{J(T)} d^n z\, e^{-S(z)} \\ &= \int_{\mathbb{R}^n} d^n x\, \det\left(\frac{\partial z(T,x)}{\partial x}\right) e^{-S(z(T,x))} \\ &= \int_{\mathbb{R}^n} d^n x\, e^{-\underbrace{\left[S(z(T,x)) - \ln \det\left(\frac{\partial z(T,x)}{\partial x}\right)\right]}_{=\, S_{eff}(x)}}. \end{aligned}$$

Thanks to the gradient flow, the sign problem of S_{eff} is expected to be milder than S.

$\Rightarrow$ Apply MC + reweighting.